Extended coupled cluster method

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EXTENDED COUPLED CLUSTER METHOD: QUANTUM MANY-BODY THEORY MADE CLASSICAL

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1. INTRODUCTION

We focus attention in this paper on how the general quantum many-body problem can be cast in the form of a variational principle for a specified action functional. After some preliminary discussion in Section 2 concerning the algebra of the many-body operators and the development of a convenient shorthand notation to describe it, we show in Section 3 how each of the configuration-interaction (CI)[1] method, the normal coupled cluster method (CCM),[2-6] and an extended version of the CCM,[7,8] can be derived by specific parametrisations of the ground-state bra and ket wavefunctions in the action functional. In each case we make contact and comparison with time-independent perturbation theory, and we discuss the various "tree-diagram" structures that emerge in each case.

As is widely appreciated by now, the CI method contains unlinked diagrams for the energy, no generalised time-ordering (g.t.o.) properties, and suffers accordingly from the size-extensivity problem.[6] By contrast, the normal CCM takes account of the linked-cluster theorem,[9,10] has a well-known g.t.o. structure ("backwards in time") which leads to connected diagrams for the energy of the normal tree structure (in which each link is a group of particle or particle-hole lines parametrised by some configuration-space index ξ), and does not suffer from the size-extensivity problem. Although evaluation of the energy does not require the bra ground state, it is needed for the expectation values of other operators, and in the normal CCM the operators parametrising the bra ground state are not linked. Practical problems can thereby still arise as for the CI method. Finally, it is shown how maximal use is made of the linked-cluster theorem in the extended CCM, and how each of the amplitudes $\sigma(\xi)$ and $\tilde{\sigma}(\xi)$ which now completely specify the bra and ket ground states, is fully linked and is hence quasi-local in the sense of obeying the usual cluster property. We point out how the extended CCM (ECCM) can also be cast in the form of generalised tree diagram structures that now have a g.t.o. property both forwards as well as backwards in time.

In view of the above properties, the remainder of this paper is concerned with the ECCM. Just as the normal CCM is intimately connected with a similarity transformation,[2] as is by now well-known, so the ECCM contains a double similarity transformation. In Section 4 we show how various matrix elements involving the double similarity transform of an arbitrary operator can be related to the functional derivatives with respect to the basic amplitudes $\sigma,\tilde{\sigma}$ of the average-value functional for the original operator. We hence show how the average values of arbitrary operator products can be evaluated. These results are applied in Section 5 to the very important case of operator commutators, and in so doing we show very explicitly how a set of generalised Poisson brackets naturally arises, and how thereby the general many-body ground-state problem can be formally mapped exactly onto the classical hamiltonian mechanics for the many-body, classical (c-number), quasi-local, configuration-space fields $\sigma(\xi)$ and $\tilde{\sigma}(\xi)$. This discussion is extended in Section 6 to show how a generalised mean-field theory can be exactly associated with the original many-body quantum theory, in terms of a set of generalised coherent states defined in some (fictitious) boson Hilbert space $\mathcal{H}^B$, which can itself be associated with the original Hilbert space $\mathcal{H}$. In this way we develop an exact correspondence between the generalised coherent states in $\mathcal{H}^B$ and the states representable in $\mathcal{H}$ via the ECCM as previously described. The quantum many-body problem in $\mathcal{H}$ is thus exactly "bosonised" into a (semiclassical) effective boson theory in $\mathcal{H}^B$ which is to be treated at the (generalised) mean-field level only. Finally, we compare this new "bosonisation" procedure with previous such methods in Section 7, where further extensions and applications of the ECCM are also briefly discussed.

2. OPERATOR ALGEBRA IN THE MANY-BODY HILBERT SPACE

It is typical of many quantum-mechanical calculations that the construction of states belonging to the full Hilbert space $\mathcal{H}$, is based on some initial or model state $|\Phi\rangle$. This is often, but not necessarily chosen to be some suitable state that the system would otherwise be in when (some part of) the interactions are turned off. We start here with such a state $|\Phi\rangle$, and assume furthermore that the algebra of all operators in $\mathcal{H}$ is spanned by the two subalgebras of creation and destruction operators defined with respect to the given model state $|\Phi\rangle$. We assume further that these two subalgebras and the state $|\Phi\rangle$ are *cyclic* in the sense that all of the ket states in $\mathcal{H}$ can be constructed from linear combinations of the states reached by operating on $|\Phi\rangle$ with the elements of the creation operator subalgebra; and similarly for the bra states with respect to the state $\langle\Phi|$.

We introduce a very convenient short-hand notation for the general creation and annihilation operators, $C^{\dagger}(\xi)$ and $C(\xi)$ respectively, where the label ξ is intended to represent a subset of any suitable complete set of general configuration-space indices. As an example, if $|\Phi\rangle$ is chosen to be the vacuum of a many-boson system, so that $a_i|\Phi\rangle = 0$ for all single-boson destruction operators a_i, then we may choose

$$C^{\dagger}(\xi) \rightarrow \prod_{i=1}^{m} (n_i!)^{-\frac{1}{2}} (a_i^{\dagger})^{n_i} \tag{1a}$$

and the configuration index $\xi \rightarrow \{n_i\}$ is a shorthand for any such set of integers $(n_1, n_2, \cdots n_m)$. Alternatively, in real space we may write

$$C^{\dagger}(\xi) \rightarrow (m!)^{-\frac{1}{2}} \prod_{i=1}^{m} a^{\dagger}(\vec{x}_i) \tag{1b}$$

and the configuration index $\xi \rightarrow (\vec{x}_1, \vec{x}_2, \cdots \vec{x}_m)$. In any case we assume

that with any such appropriate configuration space, the identity operator I in $\mathcal{H}$ can be resolved as,

$$I = |\Phi\rangle\langle\Phi| + \int' d\xi\, C^\dagger(\xi)|\Phi\rangle\langle\Phi|C(\xi)$$
$$= \int d\xi\, C^\dagger(\xi)|\Phi\rangle\langle\Phi|C(\xi) \quad , \tag{2}$$

in terms of a normalised set of creation and destruction operators,

$$\langle\Phi|C(\xi)C^\dagger(\xi')|\Phi\rangle = \delta(\xi - \xi') \ , \tag{3}$$

and where the integral over ξ in Eq.(2) must as usual be interpreted as a sum for discrete configuration-space labels. We also point out our convention in Eq.(2) that a prime on the integration symbol indicates the restriction that we include only those creation operators $C^\dagger(\xi)$ which create at least one particle. Conversely, an integration with no prime also includes the model state itself, that is $C^\dagger(0) \equiv I$ is included.

The reader should take careful note of our shorthand notation now, since it is quite vital for later formal developments. Without this compact notation, our later formulae would become very complicated. Worse still, they would be system-dependent. We note that our formalism is very general, and the extension to systems of fermions or spin-algebraic systems etc. is, at least in principle, straightforward. *However, for the purposes of the remainder of this paper, we shall henceforth restrict ourselves to bosonic systems.*

As indicated previously, we now assume that an arbitrary ket state $|K\rangle$ in $\mathcal{H}$ can be written as

$$|K\rangle = \int d\xi\, k(\xi)C^\dagger(\xi)|\Phi\rangle \ ; \ k(\xi) = \langle\Phi|C(\xi)|K\rangle \tag{4}$$

and similarly for an arbitrary bra state.

For later use we will also find it very useful to develop a notation for compounding configuration indices. We shall denote these by the ordinary symbols of addition and subtraction, e.g. $(\xi + \xi')$ and $(\xi - \xi')$, but it is clear from our prior discussion that these cannot possibly be interpreted in the usual arithmetical sense. Instead, we give the very specific definitions,

$$C^\dagger(\xi+\xi') \equiv C^\dagger(\xi)C^\dagger(\xi') \ ; \ C(\xi+\xi') = C(\xi')C(\xi)$$
$$C^\dagger(\xi-\xi')|\Phi\rangle \equiv C(\xi')C^\dagger(\xi)|\Phi\rangle; \ \langle\Phi|C(\xi-\xi') \equiv \langle\Phi|C(\xi)C^\dagger(\xi') \ . \tag{5}$$

Since the operator $C^\dagger(\xi-\xi')$ is thus, more specifically, defined to be the creation part (with respect to $|\Phi\rangle$) of the full contraction of the product $C(\xi')C^\dagger(\xi)$, it is clear that it is non-zero only when the index set ξ' is a proper subset of the index set ξ. We may similarly then define compounded expansion coefficients,

$$k(\xi+\xi') \equiv \langle\Phi|C(\xi)C(\xi')\int d\eta\, k(\eta)C^\dagger(\eta)|\Phi\rangle = \langle\Phi|C(\xi+\xi')|K\rangle \ ,$$
$$k(\xi-\xi') \equiv \langle\Phi|C(\xi)C^\dagger(\xi')\int d\eta\, k(\eta)C^\dagger(\eta)|\Phi\rangle = \langle\Phi|C(\xi-\xi')|K\rangle \ . \tag{6}$$

The reader should be warned, in case of later temptation, that these operations of addition or subtraction on the configuration indices are generally neither associative nor commutative, e.g. $k(\xi+(\xi'-\xi")) \neq k((\xi+\xi')-\xi")$;

although $k(\xi-(\xi'+\xi'')) = k((\xi-\xi')-\xi'')$. Finally, we note that a very useful form of Wick's theorem (for bosons) can be proved which, in our notation, reads as

$$C(\xi')C^{\dagger}(\xi) = \int d\eta C^{\dagger}(\xi-\eta)C(\xi'-\eta) \quad . \tag{7}$$

3. DYNAMIC VARIATIONAL PRINCIPLE AND GENERALISED TREE DIAGRAMS

For later purposes we shall not wish to restrict ourselves to hamiltonians, or their relevant subsequent transforms, that are necessarily hermitian. Hence, with complete generality we denote the ground-state bra and ket states of the exact many-body hamiltonian H as $\langle\Psi'|$ and $|\Psi\rangle$, where

$$H|\Psi\rangle = E|\Psi\rangle \; ; \; \langle\Psi'|H = E\langle\Psi'| \quad , \tag{8}$$

corresponding to ground-state energy E. If either the hamiltonian depends on time or if the system is not in equilibrium, we must use the time-dependent Schrödinger equations instead of Eq.(8). In turn, these can be formulated in terms of a *dynamic variational principle* based on an action-like (henceforth referred to as the action) functional

$$\mathcal{A} = \mathcal{A}[\Psi,\Psi'] \equiv \int dt \, \langle\Psi'(t)|(i\partial/\partial t - H)|\Psi(t)\rangle \quad . \tag{9}$$

Stationarity of $\mathcal{A}$ with respect to all variations in the independent states $|\Psi\rangle$ and $\langle\Psi'|$ (subject only to the vanishing of $|\delta\Psi\rangle$ and $\langle\delta\Psi'|$ at the implied end-points of the time-integration in Eq.(9) -- usually $t \to \pm\infty$), then gives the correct Schrödinger equations of motion,

$$\frac{\delta\mathcal{A}}{\delta\Psi'} = 0 \Rightarrow i\frac{\partial}{\partial t}|\Psi(t)\rangle = H|\Psi(t)\rangle ; \frac{\delta\mathcal{A}}{\delta\Psi} = 0 \Rightarrow -i\frac{\partial}{\partial t}\langle\Psi'(t)| = \langle\Psi'(t)|H \; . \tag{10}$$

We now show how various *parametrisations* of $\langle\Psi'|$ and $|\Psi\rangle$ lead to purely algebraic ways to generate many-body structures (diagrams) that can very usefully be cast in the form of *generalised tree diagrams*. In particular, we compare and contrast three different (potentially exact) many-body formalisms: (i) the configuration-interaction (CI) method[1], (ii) the normal coupled cluster method (CCM),[2-6] and (iii) the extended coupled cluster method (ECCM).[7,8] We shall show how the ECCM has many formal advantages over the normal CCM, just as the normal CCM has many merits over the CI method, as is by now very well known.[4,6] In the later Sections we then discuss the ECCM and some of its applications in more detail.

3·1. Configuration-Interaction Representation

In the CI method, $|\Psi\rangle$ and $\langle\Psi'|$ are parametrised as,

$$|\Psi\rangle = F|\Phi\rangle = \int d\xi\sigma_1(\xi)C^{\dagger}(\xi)|\Phi\rangle \; ; \; \langle\Psi'| = \langle\Phi|\tilde{F} = \int d\xi\,\tilde{\sigma}_1(\xi)\langle\Phi|C(\xi) \quad . \tag{11}$$

It is then easy to show that the action functional of Eq.(9) becomes,

$$\begin{aligned} \mathcal{A}[\sigma_1,\tilde{\sigma}_1] \equiv \mathcal{A}_1 &= \int dt \left\{ i\int d\xi\tilde{\sigma}_1(\xi)\dot{\sigma}_1(\xi) - \bar{H}[\sigma_1,\tilde{\sigma}_1]\right\} \\ &= \int dt \left\{ -i\int d\xi\dot{\tilde{\sigma}}_1(\xi)\sigma_1(\xi) - \bar{H}[\sigma_1,\tilde{\sigma}_1]\right\} \end{aligned} \tag{12}$$

where $\bar{H} \equiv \langle\Psi'|H|\Psi\rangle$ is specified as

$$\bar{H}_1 \equiv \bar{H}[\sigma_1,\tilde{\sigma}_1] \equiv \langle\Psi'|H|\Psi\rangle = \int d\xi \int d\xi' \langle\xi|H|\xi'\rangle \tilde{\sigma}_1(\xi)\sigma_1(\xi') ,$$
$$\langle\xi|H|\xi'\rangle = \langle\Phi|C(\xi)HC^{\dagger}(\xi')|\Phi\rangle \quad . \tag{13}$$

Requiring $\bar{H}_1$ to be stationary with respect to arbitrary small changes in $\tilde{\sigma}_1(\xi)$ and $\sigma_1(\xi')$, then yields respectively the dynamical equations,

$$i\dot{\sigma}_1(\xi) = \frac{\delta\bar{H}_1}{\delta\tilde{\sigma}_1(\xi)} \quad ; \quad i\dot{\tilde{\sigma}}_1(\xi) = -\frac{\delta\bar{H}_1}{\delta\sigma_1(\xi)} \quad . \tag{14}$$

The ground state is clearly given by the (stationary in time) equilibrium point,

$$\frac{\delta\bar{H}_1}{\delta\sigma_1(\xi)} = 0 = \frac{\delta\bar{H}_1}{\delta\tilde{\sigma}_1(\xi)} \quad . \tag{15}$$

If the hamiltonian can be split into a sum of a one-body operator (kinetic energy) part T and an interaction part V, $H = T+V$, and furthermore if the configuration space has been chosen so that the states $C^{\dagger}(\xi)|\Phi\rangle$ are eigenstates of T, then it is easily shown that

$$\langle\Psi'|T|\Psi\rangle \equiv \bar{T}[\sigma_1,\tilde{\sigma}_1] \equiv T_1 = \int d\xi\, E(\xi)\tilde{\sigma}_1(\xi)\sigma_1(\xi) + \text{const.}, \tag{16}$$

where $E(\xi)$ is the extra kinetic energy of the configuration $C^{\dagger}(\xi)|\Phi\rangle$ with respect to the model state $|\Phi\rangle$. Equation (15) may then be cast in the form,

$$\sigma_1(\xi) = -\frac{1}{E(\xi)}\frac{\delta\bar{V}_1}{\delta\tilde{\sigma}_1(\xi)} \quad ; \quad \tilde{\sigma}_1(\xi) = -\frac{1}{E(\xi)}\frac{\delta\bar{V}_1}{\delta\sigma_1(\xi)} \quad , \tag{17}$$

where the factors $E(\xi)$ appear in the usual guise of "energy denominators". Equations (17) may be regarded as the Dyson equations for the functions $\sigma_1(\xi)$ and $\tilde{\sigma}_1(\xi)$. Their solution by iteration leads to a set of terms which can be recognised as Goldstone diagrams.

The resulting CI equations, while simple, are known to have a very serious drawback for applications to many-body systems. This hinges on the fact that the diagrams for both $\sigma_1(\xi)$ and $\tilde{\sigma}_1(\xi)$ contain *disconnected* pieces. A corollary is that both sets of amplitudes are *strongly non-local* in the sense that they do not possess the cluster property, e.g. $\sigma_1(\vec{x}_1,\vec{x}_2,\vec{x}_3) \not\to 0$ as $\vec{x}_3$ is removed very far from both $\vec{x}_1$ and $\vec{x}_2$. Although the CI method is in principle exact, in practice it needs to be truncated, and the disconnected (unlinked) nature of the amplitudes then leads to the well-known "size-consistency" or "size-extensivity" problem.[6] A further, more minor, drawback to the method is that there is no manifest normalisation built into it, viz. $\langle\Psi'|\Psi\rangle \neq 1$ necessarily (although Eq.(10) does guarantee that $(d/dt)\langle\Psi'|\Psi\rangle = 0$). Nevertheless, the CI method has often been used in few-body applications, especially to problems in the realm of quantum chemistry.

3·2. Normal Coupled Cluster Representation

The roots of the coupled cluster method (CCM) date back to Hubbard[9] who realised that the problems associated with the disconnected nature of the operator F in Eq.(11) could be rectified by writing F in the form $F = \exp(S)$, where S contains only linked terms; and whence follows the linked cluster theorem of Goldstone[10] for the ground-state energy. So long

as we are only interested in the ground state energy E, the static Schrödinger equation (8) may be written in the form,[2]

$$e^{-S}He^{S}|\Phi\rangle = E|\Phi\rangle \quad . \tag{18}$$

The overlap of Eq.(18) with $\langle\Phi|$ gives E itself, while the overlaps with the states $\langle\Phi|C(\xi)$ give the normal ground-state CCM hierarchy of equations that fully determine the operator S. When we need expectation values of operators other than H, it becomes necessary also to involve the state $\langle\Psi'|$. In the normal CCM, the parametrisation of the bra and ket ground states is given as,

$$\begin{aligned} |\Psi\rangle &= e^{S}|\Phi\rangle \;;\; S = \int' d\xi\sigma_2(\xi)C^{\dagger}(\xi) \\ \langle\Psi'| &= \langle\Phi|\Omega e^{-S};\; \Omega = 1+\int' d\xi\tilde{\sigma}_2(\xi)C(\xi) \quad , \end{aligned} \tag{19}$$

which may be compared with the equivalent CI expressions (11). It is immediately clear from Eq.(19) that our ground states are manifestly normalised, $\langle\Psi'|\Psi\rangle = 1$. Inserting from Eq.(19) into the action functional of Eq.(9) leads to the expression,

$$\mathcal{A}[\sigma_2,\tilde{\sigma}_2] \equiv \mathcal{A}_2 = \int dt \left\{ i\int' d\xi\tilde{\sigma}_2(\xi)\dot{\sigma}_2(\xi) - \bar{H}[\sigma_2,\tilde{\sigma}_2]\right\} \;; \tag{20}$$

$$\bar{H}[\sigma_2,\tilde{\sigma}_2] \equiv \bar{H}_2 \equiv \langle\Psi'|H|\Psi\rangle = \langle\Phi|\Omega e^{-S}He^{S}|\Phi\rangle \quad , \tag{21}$$

and where we note that the fact that the creation and annihilation subalgebras are Abelian makes the taking of the relevant derivatives above very easy.

We may now define an *average-value functional* for an arbitrary operator Θ as,

$$\begin{aligned} \langle\Psi'|\Theta|\Psi\rangle &\equiv \bar{\Theta}[\sigma_2,\tilde{\sigma}_2] \equiv \bar{\Theta}_2 = \langle\Phi|\Omega e^{-S}\Theta e^{S}|\Phi\rangle \\ &= \sum_{n=0}^{N}\frac{1}{n!}\langle\Phi|\Omega[\cdots[[\Theta,S],S],\cdots S]|\Phi\rangle \end{aligned} \tag{22}$$

where in the well-known nested commutator expansion employed in Eq.(22), the operator S appears n times. If Θ is a symmetrised sum of j-body operators, then the upper limit on the sum becomes N = 2j. Formally we may write,

$$\begin{aligned} \bar{\Theta}[\sigma_2,\tilde{\sigma}_2] = \sum_{m=0}^{1}\sum_{n=0}^{N}\frac{1}{m!n!}\int d\xi_1\int' d\xi_1'\cdots\int' d\xi_n'\langle\xi_m|\Theta|\xi_1'\cdots\xi_n'\rangle \\ \times\tilde{\sigma}_2(\xi_1)\sigma_2(\xi_1')\cdots\sigma_2(\xi_n'), \end{aligned} \tag{23}$$

where, by comparison with Eq.(22), the matrix elements may be written schematically as

$$\langle\xi_1|\Theta|\xi_1'\cdots\xi_n'\rangle = \langle\Phi|C(\xi_1)\Theta C^{\dagger}(\xi_1')\cdots C^{\dagger}(\xi_n')|\Phi\rangle_{\mathcal{L}} \quad , \tag{24}$$

and where the suffix $\mathcal{L}$ on these matrix elements indicates the very definite linked structure implied by Eq.(22).

With this notation, the stationarity of $\mathcal{A}_2$ with respect to small variations in $\sigma_2(\xi)$ and $\tilde{\sigma}_2(\xi)$ then yields dynamical equations of precisely the same form as in the CI equations (14), but with all (CI) indices 1 replaced by (normal CCM) indices 2. At the equilibrium point, the ground state is again similarly given as in Eq.(15), which equations now reduce to the form,

$$\langle\Phi|C(\xi)e^{-S}He^{S}|\Phi\rangle = 0 \quad ; \quad \xi \neq 0$$
$$\langle\Phi|\Omega[e^{-S}He^{S}, C^{\dagger}(\xi)]|\Phi\rangle = 0 \quad , \tag{25}$$

which determine the static amplitudes $\sigma_2(\xi)$ and $\tilde{\sigma}_2(\xi)$. We find that the Dyson equations for $\sigma_2, \tilde{\sigma}_2$ can again be put in similar form to the CI equations (17), but a big difference now arises from the replacement $\overline{V}_1 \rightarrow \overline{V}_2$. Thus in the present case the resulting diagrams for the energy are fully connected, as indeed are the diagrams for $\sigma_2(\xi)$ as expected from our earlier remarks on the linked-cluster theorem. However, $\tilde{\sigma}_2(\xi)$ still contains disconnected terms, and remains problematic. Of course if we restrict ourselves to the energy, then the amplitudes $\tilde{\sigma}_2(\xi)$ are not needed, as already mentioned. However, problems still remain for the expectation values of arbitrary operators.

Very related to the above discussion is the concept of *"generalised time ordering"* (g.t.o.), which is a useful tool for classifying and combining classes of Goldstone diagrams.[11,7] This technique is based on the factorisation property of disjoint sets of legs of a Goldstone diagram, and leads to the factorisation of corresponding energy denominators across such legs when all permitted time orderings are included. The normal CCM generates diagrams for the energy with a g.t.o. in the "downward" direction (i.e. backwards in time) only. The diagrams for the expectation value of the hamiltonian can thereby be represented by what we now call *"normal g.t.o. trees"* or *"normal CCM trees"*. These are diagrams which "branch out" in the downward direction only (-- thus resembling the root system of a real tree rather than the visible tree structure!). As explained elsewhere,[7] each link or branch (i.e., root!) in such a diagram corresponds to a definite set of particle/hole lines associated with the configuration ξ of the corresponding state $C^{\dagger}(\xi)|\Phi\rangle$. If such a (downward) tree diagram for the energy (the totality of which give the normal CCM expression), is divided into two by cutting one link, the lower part (which constitutes a diagram associated with some amplitude $\sigma_2(\xi)$) will always be linked, whereas the upper part (which constitutes a diagram for the corresponding amplitude $\tilde{\sigma}_2(\xi)$) may be unlinked. For further details we refer the interested reader to the by now quite extensive literature on the normal CCM and its applications.[4-6,12-15]

3·3. Extended Coupled Cluster Representation

For reasons already alluded to above, the normal CCM has been almost wholly concerned with energy calculations. There are virtually no calculations involving average-value properties of other operators. In such cases, the unlinked nature of the operator Ω (or equivalently its amplitudes $\tilde{\sigma}_2(\xi)$) may well lead to computational difficulties in the case of practical (i.e., truncated) calculations. Just as in passing from the CI method to the normal CCM we cured the $\sigma_1(\xi)$ of their disconnectedness by their replacement with $\sigma_2(\xi)$, so the extended CCM (ECCM) aims to cure the remaining disconnectedness in $\tilde{\sigma}_2(\xi)$. This is achieved by the following ECCM parametrisation,

$$|\Psi\rangle = e^{S}|\Phi\rangle \quad ; \quad S = \int' d\xi\, s(\xi)C^{\dagger}(\xi)$$
$$\langle\Psi'| = \langle\Phi|e^{S''}e^{-S} \quad ; \quad S'' = \int' d\xi\, \tilde{\sigma}_3(\xi)C(\xi) \quad , \tag{26}$$

which may be compared with its normal CCM counterpart in Eq.(19). Just as in the normal CCM, the coefficients $\tilde{\sigma}_2(\xi)$ are the (unlinked) average values of the creation operators, $\tilde{\sigma}_2(\xi) = \langle\Psi'|C^{\dagger}(\xi)|\Psi\rangle$, so now it can be shown that the linked parts of these averages are precisely the new amplitudes $\tilde{\sigma}_3(\xi)$. Again, the ground states are trivially observed to be manifestly normalised, $\langle\Psi'|\Psi\rangle = 1$. An average-value functional of an arbitrary operator Θ now

takes the form,

$$\bar{\Theta} \equiv \langle\Psi'|\Theta|\Psi\rangle = \langle\Phi|\hat{\Theta}|\Phi\rangle \quad , \tag{27}$$

in terms of the (doubly) similarity-transformed operator $\hat{\Theta}$,

$$\hat{\Theta} \equiv e^{S''}e^{-S}\Theta e^{S}e^{-S''} \quad . \tag{28}$$

Finally in the ECCM, it turns out to be very convenient to define a new operator Σ,

$$\Sigma \equiv \int' d\xi\, \sigma_3(\xi)C^{\dagger}(\xi) \quad ; \quad \sigma_3(\xi) \equiv \langle\Phi|C(\xi)e^{S''}S|\Phi\rangle \quad , \tag{29}$$

which has an inverse transformation,

$$S|\Phi\rangle = e^{-S''}\Sigma|\Phi\rangle \quad ; \quad s(\xi) = \langle\Phi|C(\xi)e^{-S''}\Sigma|\Phi\rangle \quad . \tag{30}$$

Insertion of the above parametrisation into the action functional of Eq.(9) gives again a form analogous to that in Eqs.(12) and (20),

$$\mathcal{A}[\sigma_3,\tilde{\sigma}_3] \equiv \mathcal{A}_3 = \int dt\, \{i\int' d\xi\tilde{\sigma}_3(\xi)\dot{\sigma}_3(\xi) - \bar{H}[\sigma_3,\tilde{\sigma}_3]\} \quad . \tag{31}$$

The variational principle again leads to the dynamic equations,

$$i\dot{\sigma}_3(\xi) = \frac{\delta\bar{H}_3}{\delta\tilde{\sigma}_3(\xi)} \quad ; \quad i\dot{\tilde{\sigma}}_3(\xi) = -\frac{\delta\bar{H}_3}{\delta\sigma_3(\xi)} \quad . \tag{32}$$

The expression for $\bar{H}_3 \equiv \bar{H}[\sigma_3,\tilde{\sigma}_3]$ is now more complicated than before. The general form of an arbitrary[3] average-value functional $\bar{\Theta}$ can now be shown to be given by,

$$\bar{\Theta}[\sigma_3,\tilde{\sigma}_3] \equiv \bar{\Theta}_3 = \sum_{m,n} \frac{1}{m!n!} \int'd\xi_1\cdots\int'd\xi_m\int'd\xi'_1\cdots\int'd\xi'_n\langle\xi_1\cdots\xi_m|\Theta|\xi'_1\cdots\xi'_n\rangle \times \tilde{\sigma}(\xi_1)\cdots\tilde{\sigma}(\xi_m)\sigma(\xi'_1)\cdots\sigma(\xi'_n) \quad , \tag{33}$$

in which the matrix elements, expressed schematically by the expression,

$$\langle\xi_1\cdots\xi_m|\Theta|\xi'_1\cdots\xi'_n\rangle = \langle\Phi|C(\xi_1)\cdots C(\xi_m)\Theta C^{\dagger}(\xi'_1)\cdots C^{\dagger}(\xi'_n)|\Phi\rangle_{\mathcal{DL}} \tag{34}$$

have a very definite linked ($\mathcal{DL}$) structure, as can be found by explicit construction, and as explained in detail elsewhere.[7] We note here only that the matrix elements of Eq.(34) are not all independent, in the sense that one may find definite recursion relations between them. Particularly useful in this respect is the identity,

$$\frac{\delta\bar{\Theta}_3}{\delta\tilde{\sigma}_3(\xi+\xi')} = \frac{\delta^2\bar{\Theta}_3}{\delta\tilde{\sigma}_3(\xi)\delta\tilde{\sigma}_3(\xi')} + \int' d\eta\left[\sigma_3(\xi+\eta)\frac{\delta^2\bar{\Theta}_3}{\delta\sigma_3(\eta)\delta\tilde{\sigma}_3(\xi')} + \frac{\delta^2\bar{\Theta}_3}{\delta\tilde{\sigma}_3(\xi)\delta\sigma_3(\eta)}\sigma_3(\eta+\xi')\right] + \int' d\eta\int' d\eta'\sigma_3(\xi+\eta)\frac{\delta^2\bar{\Theta}_3}{\delta\sigma_3(\eta)\delta\sigma_3(\eta')}\sigma_3(\eta'+\xi') \quad . \tag{35}$$

Such relations as Eq.(35) in the ECCM are most easily proven by starting with the average value functional $\bar{\Theta}$ written as a functional of the operators S'' and S; and then making the change of 'variables' to the operators S'' and Σ in the usual partial differential sense, as discussed further in Section 4.

As usual, the energy functional $\bar{H} \equiv \langle\Psi'|H|\Psi\rangle$ now plays the particularly important role, through Eq.(32), of determining the dynamics of the amplitudes $\sigma_3(\xi)$ and $\tilde{\sigma}_3(\xi')$, and their equilibrium values. The kinetic energy operator T has an average value functional which, after some algebra, can be expressed in terms of these amplitudes as,

$$\bar{T}[\sigma_3,\tilde{\sigma}_3] = \langle\Phi|S''T\Sigma|\Phi\rangle = \text{const.} + \int' d\xi E(\xi)\tilde{\sigma}_3(\xi)\sigma_3(\xi) \quad . \tag{36}$$

Comparison with Eq.(16), and the discussion following it, again shows that at equilibrium the values of $\sigma_3,\tilde{\sigma}_3$ represent the contributions of definite classes of Goldstone diagrams. These may again be conveniently classified in terms of *extended g.t.o. trees*.[7] By comparison with the normal CCM, these extended CCM tree diagrams now branch upwards as well as downwards at any vertex. The average value functional for an arbitrary operator may then uniquely be expressed in terms of such extended g.t.o. tree diagrams. A consequence is that if any such extended tree diagram for the energy is divided into two by cutting any single link, both the top part (which is a diagram for $\tilde{\sigma}_3$) and the bottom part (which is a diagram for σ_3) now separately remain connected diagrams. In this way, now *all* of our basic amplitudes $\sigma_3(\xi)$ and $\tilde{\sigma}_3(\xi)$ in the ECCM are quasi-local in the sense that they obey the *cluster property*, namely that if any subset of the particles incorporated in the configuration-space labelling ξ is removed infinitely far from the remainder, the amplitude goes to zero.

In the remainder of this paper we now deal only with the extended CCM and investigate some of its consequences and uses. We therefore now drop the suffices 3, and henceforth rename $\tilde{\sigma}_3(\xi) \rightarrow \tilde{\sigma}(\xi)$; $\sigma_3(\xi) \rightarrow \sigma(\xi)$.

4. FUNCTIONAL DERIVATIVES AND MATRIX ELEMENTS

Neither the normal nor extended version of the CCM is manifestly hermitian. In the ECCM with which we are now concerned, this ultimately derives from the fact that the (double) similarity transformations which generate the ket and bra ground states are not unitary. Thus the formalism is actually a *biorthogonal* formulation of the many-body problem, and the functional $\bar{\Theta}$ of Eq.(27), for an arbitrary operator Θ, represents the real expectation value functional, in view of the definite normalisation $\langle\Psi'|\Psi\rangle = 1$.

For further development of the ECCM formalism, we will have need for various matrix elements involving the doubly similarity-transformed operator $\hat{\Theta}$ of Eq.(28), and we now point out and exploit the intimate connection between such matrix elements and the functional derivatives of the average-value functional $\bar{\Theta}$. It is clear from our earlier discussion that it is easiest to compute $\bar{\Theta}$ in the first place as a functional of the operators S and S'',

$$\bar{\Theta} = \langle\Phi|e^{S''}e^{-S}\,\Theta e^{S}|\Phi\rangle \quad , \tag{37}$$

where we have used Eqs.(27) and (28), and the fact that S'' is built only from annihilation operators, as in Eq.(26). From Eq.(37) we may thus express the average-value functional in the form $\bar{\Theta} = \bar{\bar{\Theta}}[s,\tilde{\sigma}]$, using Eqs.(26), where the double-bar notation simply reminds us of the functional arguments. It is then trivial to see directly from Eq.(37) that the first-order functional derivatives in this representation are given by,

$$\frac{\delta\bar{\bar{\Theta}}}{\delta\tilde{\sigma}(\xi)} = \langle\Phi|C(\xi)\hat{\Theta}|\Phi\rangle \quad ; \quad \frac{\delta\bar{\bar{\Theta}}}{\delta s(\xi)} = \langle\Phi|e^{S''}e^{-S}[\Theta,C^{\dagger}(\xi)]e^{S}|\Phi\rangle \quad . \tag{38}$$

Finally, we may "change variables" from the operators S,S'' to Σ,S'' using

Eq.(29) to give equivalently $\bar{\Theta} \rightarrow \bar{\Theta}[\sigma,\tilde{\sigma}] \equiv \bar{\bar{\Theta}}[s,\tilde{\sigma}]$. Making use of the usual chain rule of partial differentiation, we readily find,

$$\frac{\delta\bar{\bar{\Theta}}}{\delta\tilde{\sigma}(\xi)} = \frac{\delta\bar{\Theta}}{\delta\tilde{\sigma}(\xi)} + \int' d\xi'\sigma(\xi+\xi')\frac{\delta\bar{\Theta}}{\delta\sigma(\xi')} \; ; \; \frac{\delta\bar{\bar{\Theta}}}{\delta s(\xi)} = \int' d\xi'\omega(\xi-\xi')\frac{\delta\bar{\Theta}}{\delta\sigma(\xi')} \; , \quad (39)$$

where we have used the notation of Eqs.(5) and (6) to compound the configuration space indices; and where the amplitude $\omega(\xi)$ and a comparable amplitude $\bar{\omega}(\xi)$ needed later, are defined as,

$$\omega(\xi) \equiv \langle\Phi|e^{S''}C^{\dagger}(\xi)|\Phi\rangle \; ; \; \bar{\omega}(\xi) \equiv \langle\Phi|e^{-S''}C^{\dagger}(\xi)|\Phi\rangle \quad . \quad (40)$$

These latter amplitudes are easily seen to obey the orthogonality relations,

$$\int d\eta\bar{\omega}(\xi-\eta)\omega(\eta-\xi') = \delta(\xi-\xi') = \int d\eta\omega(\xi-\eta)\bar{\omega}(\eta-\xi') \quad . \quad (41)$$

We also note in passing that our previous Eq.(35) is proven by making repeated use of Eq.(39) together with the trivial relation $\delta^2\bar{\bar{\Theta}}/\delta\tilde{\sigma}(\xi)\delta\tilde{\sigma}(\xi') = \delta\bar{\bar{\Theta}}/\delta\tilde{\sigma}(\xi+\xi')$, which follows immediately from Eq.(38).

The combination of Eqs.(38) and (39) immediately gives that for an arbitrary operator A,

$$\langle\Phi|C(\xi)\hat{A}|\Phi\rangle = \frac{\delta\bar{A}}{\delta\tilde{\sigma}(\xi)} + \int' d\xi'\sigma(\xi+\xi')\frac{\delta\bar{A}}{\delta\sigma(\xi')} \; ; \; \xi \neq 0 \quad . \quad (42)$$

Relatively straightforward algebra using the above relations and judicious insertions of the identity operator from Eq.(2), also leads to other comparable expressions involving matrix elements of the operator $\hat{A}$ being able to be written in terms of functional derivatives of the average-value functional $\bar{A} = \bar{A}[\sigma,\tilde{\sigma}]$. As a further example, we simply quote the result (valid for $\xi \neq 0$),

$$\langle\Phi|\hat{A}C^{\dagger}(\xi)|\Phi\rangle = \frac{\delta\bar{A}}{\delta\sigma(\xi)} + \int' d\eta\,\frac{\delta\bar{A}}{\delta\tilde{\sigma}(\eta)}L(\eta\xi) + \int' d\eta\int' d\eta'\frac{\delta\bar{A}}{\delta\sigma(\eta)}\sigma(\eta+\eta')L(\eta'\xi) \; , \quad (43)$$

where the function $L(\xi\xi') = L(\xi'\xi)$ is defined as,

$$L(\xi\xi') = \int d\eta\int d\eta'\omega(\eta+\eta')\bar{\omega}(\xi-\eta)\bar{\omega}(\xi'-\eta') = \langle\Phi|e^{S''}C^{\dagger}(\xi)C^{\dagger}(\xi')|\Phi\rangle \quad . \quad (44)$$

In a similar fashion one may evaluate higher matrix elements in terms of higher-order functional derivatives, e.g. the matrix element $\langle\Phi|C(\xi)\hat{A}C^{\dagger}(\xi')|\Phi\rangle$ will involve second-order derivatives. Evaluation of these higher elements is often facilitated by a judicious use of Wick's theorem in the form of Eq.(7).

4·1. Average Values of Operator Products

As a nice example of the above techniques we now turn to the very important topic of the representation in the ECCM of operator products. It is clear that products of operators transform under the double similarity transformation of Eq.(28) into the corresponding product of transformed operators, and therefore that their average values can be represented in the ECCM as,

$$\langle\Psi'|\Theta_1\Theta_2\cdots\Theta_n|\Psi\rangle = \langle\Phi|\hat{\bar{\Theta}}_1\hat{\bar{\Theta}}_2\cdots\hat{\bar{\Theta}}_n|\Phi\rangle \quad . \quad (45)$$

If, on the right-hand side of Eq.(45), one inserts the identity operator from Eq.(2) between each adjacent pair of operators, we may thereby express such average values in terms of first or second functional derivatives of the average values of the individual operators. For present purposes we restrict ourselves to what is in any case the most important example of the product of

two operators. In this case we need only first-order derivatives, and Eqs. (42) and (43) suffice. In this way we may easily evaluate the average value $\overline{AB} \equiv \langle\Psi'|AB|\Psi\rangle \equiv \langle AB\rangle$ as,

$$\overline{AB} = \overline{A}\cdot\overline{B} + \int' d\xi \int' d\xi' \left[\frac{\delta\overline{A}}{\delta\sigma(\xi)} \frac{\delta\overline{B}}{\delta\sigma(\xi')} X_{11}(\xi\xi') + \frac{\delta\overline{A}}{\delta\sigma(\xi)} \frac{\delta\overline{B}}{\delta\tilde{\sigma}(\xi')} X_{12}(\xi\xi') + \frac{\delta\overline{A}}{\delta\tilde{\sigma}(\xi)} \frac{\delta\overline{B}}{\delta\sigma(\xi')} X_{21}(\xi\xi') + \frac{\delta\overline{A}}{\delta\tilde{\sigma}(\xi)} \frac{\delta\overline{B}}{\delta\tilde{\sigma}(\xi')} X_{22}(\xi\xi') \right] \tag{46}$$

where the X-coefficients are given by the expressions

$$X_{11}(\xi\xi') = X_{11}(\xi'\xi) = \sigma(\xi+\xi') + \int' d\eta \int' d\eta' \sigma(\xi+\eta) L(\eta\eta') \sigma(\eta'+\xi'),$$
$$X_{22}(\xi\xi') = X_{22}(\xi'\xi) = L(\xi\xi'), \tag{47}$$
$$X_{12}(\xi\xi') = \delta(\xi-\xi') + \int' d\eta \sigma(\xi+\eta) L(\eta\xi') \; ; \; X_{21}(\xi\xi') = \int' d\eta L(\xi\eta)\sigma(\eta+\xi') \; .$$

5. COMMUTATORS AND GENERALISED POISSON BRACKETS

As a particularly important application of the results of Section 4·1, we now consider the expectation value of the *commutator* of two operators. In view of the high degree of symmetry exhibited in Eq.(47) by the X-coefficients, there is a considerable consequent simplification in this regard. We find,

$$\langle\Psi'|AB - BA|\Psi\rangle \equiv \langle[A,B]\rangle = i\{\overline{A},\overline{B}\} \; , \tag{48}$$

where the *generalised Poisson bracket* $\{\overline{A},\overline{B}\}$ is defined as,

$$i\{\overline{A},\overline{B}\} \equiv \int' d\xi \left[\frac{\delta\overline{A}}{\delta\sigma(\xi)} \frac{\delta\overline{B}}{\delta\tilde{\sigma}(\xi)} - \frac{\delta\overline{B}}{\delta\sigma(\xi)} \frac{\delta\overline{A}}{\delta\tilde{\sigma}(\xi)} \right] \; . \tag{49}$$

We can make these results even more suggestive by choosing as new basic (quasi-local) field variables, the *generalised fields* $\phi(\xi)$ and their canonically conjugate *generalised momentum densities* $\pi(\xi)$, defined as,

$$\phi(\xi) \equiv 2^{-\frac{1}{2}}[\sigma(\xi) + \tilde{\sigma}(\xi)] \; ; \; \pi(\xi) \equiv 2^{-\frac{1}{2}} i[\tilde{\sigma}(\xi) - \sigma(\xi)] \; . \tag{50}$$

In this way we can re-define our average values $\langle A\rangle \equiv \overline{A} \rightarrow \overline{A}[\phi,\pi]$, in terms of which Eq.(49) becomes

$$\{\overline{A},\overline{B}\} \equiv \int' d\xi \left[\frac{\delta\overline{A}}{\delta\phi(\xi)} \frac{\delta\overline{B}}{\delta\pi(\xi)} - \frac{\delta\overline{A}}{\delta\pi(\xi)} \frac{\delta\overline{B}}{\delta\phi(\xi)} \right] \tag{51}$$

The equations of motion (32) for the amplitudes $\sigma,\tilde{\sigma}$ are thereby re-cast into the form,

$$\dot{\phi}(\xi) = \frac{\delta\overline{H}}{\delta\pi(\xi)} = \{\phi(\xi),\overline{H}\} \; ; \; \dot{\pi}(\xi) = -\frac{\delta\overline{H}}{\delta\phi(\xi)} = \{\pi(\xi),\overline{H}\} \; . \tag{52}$$

Finally, for an arbitrary, intrinsically time-dependent operator $A(t)$, it is easy to show using Eqs.(52) that the equation of motion for its average-value functional $\langle A\rangle = \overline{A}[\phi,\pi;t]$ is,

$$\frac{d\overline{A}}{dt} = \left\langle \frac{\partial A}{\partial t} \right\rangle + \{\overline{A},\overline{H}\} = \left\langle \frac{\partial A}{\partial t} \right\rangle + \frac{1}{i}\langle[A,H]\rangle \; . \tag{53}$$

Equation (53) shows both that the equation of motion is indeed the proper quantum-mechanical one, and that the connection to classical physics arises through a very well-defined, suitably generalised version of the *correspondence principle*.

We are thus led to the very important result that the whole of our quantum many-body problem has formally been exactly mapped onto the classical Hamiltonian mechanics for the (c-number) quasi-local fields $\phi(\xi)$ and $\pi(\xi)$ which are themselves functions in the many-body configuration space labelled by the indices ξ. In this way we can take over (or suitably extend) the whole of the classical formalism to describe (*exactly*, in principle, if no truncations are made) the quantum many-body system. In particular we can make easy contact with such things as *conservation laws* and the associated *sum rules*, through the corresponding Noether currents.

6. EXACT BOSONISATION AND GENERALISED COHERENT STATES

It comes as no surprise that the ECCM when truncated at its lowest obvious level of approximation (-- namely, the so-called SUB1 approximation wherein in the expansions (26) and (29) for S'' and Σ, the 'sums over configurations' are restricted to one-body (i.e. one particle or one particle-hole) configurations ξ), is precisely equal to the *mean field theory* or semiclassical approximation.[7] For the bosonic systems which have mainly been emphasised here, this is precisely the ordinary *coherent-state approximation* (while for fermionic systems it is just the Hartree-Fock approximation). We briefly remind the reader how the mean field approximation for bosons can be expressed in terms of the (classical) atomic or ordinary coherent states of Glauber.[16,17] In terms of a complete set of our original single-boson creation operators in $\mathcal{H}$, say $a^{\dagger}(\vec{x})$, (and see the discussion surrounding Eqs. (1a,b)), the Glauber coherent states are defined as

$$|\gamma\rangle = e^{\Gamma}|\phi\rangle \quad ; \quad \Gamma = \int d\vec{x}[\phi(\vec{x})a^{\dagger}(\vec{x}) - \phi^{*}(\vec{x})a(\vec{x})] = -\Gamma^{\dagger} \quad , \tag{54}$$

where $\phi(\vec{x})$ and its complex conjugate $\phi^{*}(\vec{x})$ are scalar (i.e. c-number) fields, and with $|\phi\rangle$ the vacuum, $a(\vec{x})|\phi\rangle = 0$, as before. It is straightforward to show that these states are eigenstates of the destruction operator $a(\vec{x})$,

$$a(\vec{x})e^{\Gamma}|\phi\rangle = \phi(\vec{x})e^{\Gamma}|\phi\rangle \quad ; \quad \langle\phi|e^{-\Gamma}a^{\dagger}(\vec{x}) = \phi^{*}(\vec{x})\langle\phi|e^{-\Gamma} \quad . \tag{55}$$

We can then also use Eq.(55) to show rather easily that the expectation value of a suitably normal-ordered arbitrary operator $\Theta = :\Theta[a,a^{\dagger}]:$ in these coherent states is just given by replacing the field operators $a(\vec{x}), a^{\dagger}(\vec{x})$ in the functional by their c-number coherent-state expectation values $\phi(\vec{x})$, $\phi^{*}(\vec{x})$ respectively:

$$\langle\Theta\rangle_{\Gamma} \equiv \langle\phi|e^{-\Gamma} : \Theta[a,a^{\dagger}] : e^{\Gamma}|\phi\rangle = \Theta[\phi,\phi^{*}] \quad . \tag{56}$$

In particular, the static mean field approximation is obtained by minimising $\langle H\rangle_{\Gamma}$ with respect to the one-body fields $\phi(\vec{x}), \phi^{*}(\vec{x})$.

In the light of the discussion in the previous Section, it is now natural to enquire whether our entire formalism can also be *exactly* recast as a *generalised mean field theory* in terms of a well-defined set of (fictitious) *ideal coherent bosons*, whose appropriate expectation values (defined suitably in their own Hilbert space) equal the (many-body) "classical" fields $\sigma, \tilde{\sigma}$. The basic configuration space operators $C(\xi)$, $C^{\dagger}(\xi)$ are definitely not candidates for the annihilation and creation operators associated with these ideal bosons, both because their expectation values are generally much more complicated functionals of $\sigma(\xi)$ and $\tilde{\sigma}(\xi)$, and because their commutation relations are also generally not those of ideal bosons. Instead, we simply attempt to map the original many-body Hilbert space $\mathcal{H}$ onto some fictitious boson Hilbert space $\mathcal{H}^{B}$. In view of the biorthogonal nature of our previous formulation, we now postulate the existence in $\mathcal{H}^{B}$ of vacuum states $|\Phi_{B}\rangle$ and $\langle\Phi'_{B}|$, and ideal boson operators $A(\xi)$, $\tilde{A}(\xi)$ associated with each configuration ξ, such that

$$[A(\xi),A(\xi')] = 0 = [\tilde{A}(\xi),\tilde{A}(\xi')] \;;\; [A(\xi),\tilde{A}(\xi')] = \delta(\xi-\xi'),$$
$$A(\xi)|\Phi_B> = 0 = <\Phi'_B|\tilde{A}(\xi) \quad . \tag{57}$$

Furthermore, for every operator Θ in $\mathcal{H}$ we now associate its *boson image* Θ^B in $\mathcal{H}^B$, defined as:

$$\Theta^B \equiv \sum_{m,n} \frac{1}{m!n!} \int' d\xi_1 \cdots \int' d\xi_m \int' d\xi'_1 \cdots \int' d\xi'_n <\xi_1 \cdots \xi_m|\Theta|\xi'_1 \cdots \xi'_n>$$
$$\times \tilde{A}(\xi_1) \cdots \tilde{A}(\xi_m) A(\xi'_1) \cdots A(\xi'_n), \tag{58}$$

by analogy to Eq.(33), and with matrix elements exactly as specified in Eq. (34). By analogy with Eq.(54) it seems reasonable to consider a set of *generalised coherent states* (or, more properly, bi-coherent states) in $\mathcal{H}^B$, defined as

$$|\Psi_B> \equiv e^G|\Phi_B> \;;\; <\Psi'_B| \equiv <\Phi'_B|e^{-G}$$
$$G \equiv \int' d\xi[\sigma(\xi)\tilde{A}(\xi) - \tilde{\sigma}(\xi)A(\xi)] \quad , \tag{59}$$

which are to be interpreted as the images in $\mathcal{H}^B$ of the corresponding states $|\Psi>$ and $<\Psi'|$ in $\mathcal{H}$. The generalised coherent-state expectation value of Θ^B can be shown, by precise analogy with our previous atomic coherent state result of Eq.(56), to be identically equal to the earlier expression in Eq. (33),

$$<\Phi'_B|e^{-G}\Theta^B e^G|\Phi_B> = \bar{\Theta}[\sigma,\tilde{\sigma}] \quad . \tag{60}$$

Finally, we are led to consider the generalised coherent-state action functional $\mathcal{A}^B$, defined in $\mathcal{H}^B$ to be the image of the action $\mathcal{A}$ of Eq.(9) in $\mathcal{H}$,

$$\mathcal{A}^B = \int dt\, <\Phi'_B|e^{-G(t)}(i\partial/\partial t - H^B)e^{G(t)}|\Phi_B> \quad . \tag{61}$$

By making use of the result,

$$e^{-G}\frac{\partial}{\partial t}e^G = \int' d\xi\{\dot{\sigma}(\xi)\tilde{A}(\xi) - \dot{\tilde{\sigma}}(\xi)A(\xi) + \tfrac{1}{2}[\dot{\sigma}(\xi)\tilde{\sigma}(\xi) - \sigma(\xi)\dot{\tilde{\sigma}}(\xi)]\} \quad , \tag{62}$$

which follows from Eqs.(59) and (57), we finally find the result that $\mathcal{A}^B$ has an identical form to our earlier results in Eqs.(12) and (20), and most particularly in Eq.(31);

$$\mathcal{A}^B = \int dt\, \{i\int' d\xi\tilde{\sigma}(\xi)\dot{\sigma}(\xi) - \bar{H}[\sigma,\tilde{\sigma}]\} \quad . \tag{63}$$

Hence, a variational principle in $\mathcal{H}^B$ applied to the action $\mathcal{A}^B$, *exactly* reproduces our previous *exact* equations of motion (32) in $\mathcal{H}$ for the ECCM. These results are discussed further in Section 7.

7. SUMMARY AND DISCUSSION

We have shown how a variational principle for our action functional of Eq.(9) enables quantum many-body theory to be written in the form of classical hamiltonian mechanics for the many-body (c-number) configuration-space amplitudes $\sigma,\tilde{\sigma}$ for each of the CI method, the normal CCM and the extended CCM. Only in the latter case are all of these fields quasi-local in the sense of obeying the cluster property. In any realistic calculation, each of these methods must be truncated, e.g. in the so-called SUBn approximation by restricting the configuration indices ξ to at most n particles (or particle-hole pairs). In the CI method, the limbs of the associated CI trees would need to be very thick (large n), unless the interaction is so weak that low-order perturbation theory suffices. By contrast, the normal and extended CCM always perform such various infinite-order summations of Goldstone

diagrams, even for low n, that the CCM trees need not be so thick for good energy results.

However, the results are still in principle quite dependent on the choice of model state $|\Phi\rangle$. The normal (ground-state) CCM may miss altogether a phase of the system with some broken symmetry not built into $|\Phi\rangle$. One of us has shown[18] how this may be overcome within the normal CCM by constructing new model states $|\Phi'\rangle$, using a combination of the excited-state CCM formalism of Emrich[15] to search for *"de-excited states"* of lower energy than in the ground-state formalism discussed here, and the *maximum-overlap stability criterion* of Kümmel.[19] In the extended CCM, the hope is that the limbs of the generalised trees can again be relatively slim for good approximations, but by contrast the hope has been expressed[7] that the model state $|\Phi\rangle$ can remain the naive (symmetry-conserving) vacuum state even in the broken-symmetry phase. This is certainly true at the fermion SUB1 level, for example, where the normal SUB1 approximation does not produce the correct deformed Hartree-Fock state, whereas the extended CCM at SUB1 level does. The clear hope is that since the ECCM easily permits symmetry-breaking to be incorporated by introducing suitable symmetry-breaking amplitudes $\sigma,\tilde{\sigma}$ with a *given* $|\Phi\rangle$, it will find future applications to such *topological excitations* as vortices in liquid helium. Our formalism also permits applications to *non-equilibrium phenomena*, and to nonlinear behaviour far from equilibrium.

We turn now to the implications of our new bosonisation procedure discussed in Section 6. We note that there is a very long tradition in the bosonisation of spin-algebraic or fermionic systems. As examples of the genre we mention the methods of Holstein and Primakoff,[20] Dyson,[21] Schwinger,[22] and others;[23,24] and refer the reader to the review by Garbaczewski.[25] In most previous procedures the philosophy has been to establish an exact equivalence between the Lie algebra of the spin operators or suitably chosen pairs of fermion operators, and the Lie algebra of canonical boson operators in an ideal boson space. It usually transpires that the boson Hilbert space is too large, in the sense that physically realisable states in the original Hilbert space map only onto a *subspace* of the boson image space. The aim is that with a judicious choice of mapping, the low-lying collective excitations of the original system might be treated (semi-) classically or nearly so in the mapped space, in the sense that as a zeroth approximation the ideal bosons can be treated as non-interacting. Further, one hopes that to go beyond zeroth order, the residual interactions (in the usual quantum-mechanical sense) are weak enough to be easily treated by conventional means in the boson space. Generally, however, the boson interactions are far from trivial, and the formalism is still a relatively complicated theory of interacting bosons in a projected subspace of an ideal boson space.

By contrast, our own bosonisation procedure differs in at least three ways. In the first place, no effort is made to preserve the Lie algebra. Secondly, whereas earlier bosonisation schemes have been applied only to fermion or spin systems, ours may equally be applied to boson systems. Our bosonisation procedure transforms the original boson (or other) theory to an effective boson theory which is to be used at mean-field level (with only classical interactions between the bosons). Clearly, therefore, it cannot be bosonised any further! Thirdly, whereas in the earlier bosonisation schemes, the physical states map onto a subspace of the image space $\mathcal{H}^B$, here the generalised coherent states form only a *subset* of the states in $\mathcal{H}^B$. In this way we lose *the superposition principle* in the mapped physical space. The ultimate reason for this is the strongly coherent form adopted for our ground-state trial wavefunctions in Eqs.(26), which means that only the ground state and those adiabatically excited states which are strongly collective, are easily so describable.

With regard to this latter point, it is quite possible to develop further

the ground-state ECCM to include excited states in very much the same spirit as Emrich[15] has developed the normal CCM. The upshot is that the *excited states* and their *excitation energies* can be found by solving a linear eigenvalue problem to diagonalise an operator built from second-order functional derivatives of $\overline{H}$, evaluated at the equilibrium point. Likewise, our time-dependent formalism enables us to treat the same problem via the dynamics of small oscillations around the stationary equilibrium. This dynamics is again governed by an effective hamiltonian obtained by linearising the equations of motion (32) around the stationary point. In this way we can build up a set of *generalised random phase approximation* (RPA) equations in configuration space, with two main differences from the ordinary RPA.[26] Firstly, the configuration indices ξ are arbitrary, and not restricted to just one particle (or particle-hole pair) as in ordinary RPA; and secondly, when no such truncations are made the resulting generalised RPA equations are *exact*.

Further details and applications of both the present work and the extensions mentioned above, will be published elsewhere.[27,28]

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